

# Change of $\theta$ dependence in 4D SU( $N$ ) gauge theories across the deconfinement transition

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We study the dependence of 4D SU( $N$ ) gauge theories on the topological  $\theta$  term at finite temperature  $T$ . We exploit the lattice formulation of the theory, presenting numerical results for the expansion of the free energy up to  $O(\theta^6)$ , for  $N = 3$  and  $N = 6$ . Our analysis shows that the  $\theta$  dependence drastically changes across the deconfinement transition: the low- $T$  phase is characterized by a large- $N$  scaling with  $\theta/N$  as relevant variable, while in the high- $T$  phase the scaling variable is just  $\theta$  and the free energy is essentially determined by the instanton-gas approximation.

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Important physical issues of strong interactions are related to the nontrivial dependence of 4D SU( $N$ ) gauge theories on the topological parameter  $\theta$ , which appears in the Euclidean Lagrangian as

$$\mathcal{L}_\theta = \frac{1}{4} F_{\mu\nu}^a(x) F_{\mu\nu}^a(x) - i\theta \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x), \quad (1)$$

where

$$q(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x) \quad (2)$$

is the topological charge density. The presence of a nonzero  $\theta$  would break both parity and time reversal and the experimental upper bound on it is very small,  $|\theta| < 10^{-9}$  [1]. Nevertheless, the issue of  $\theta$  dependence is interesting and relevant to hadron phenomenology, an example being the so-called U(1)<sub>A</sub> problem. In the framework of the large- $N$  expansion [2–4], the nontrivial  $\theta$  dependence provides an explanation to the fact that the U(1)<sub>A</sub> symmetry of the classical theory is not realized in the hadron spectrum (see, e.g., Refs. [5, 6] for recent reviews).

In this paper we investigate the topological properties and the  $\theta$  dependence of 4D SU( $N$ ) gauge theories at finite temperature  $T$ , in particular across the deconfining temperature  $T_c$ . Such properties are known to be relevant to the thermodynamic behavior of hadronic matter. For example, the effective restoration of the U(1)<sub>A</sub> symmetry in strong interactions at finite  $T$ , and in particular around the chiral transition, is relevant to the nature of the transition itself [5, 7, 8].

As we shall better discuss in the following, one expects, on general grounds, a crossover between a low- $T$  and a high- $T$  regime for  $\theta$  dependence, characterized by different large- $N$  scalings. In particular, the high- $T$  regime should be describable by a semiclassical instanton gas picture, which instead fails in the low- $T$  regime, where  $\theta/N$  turns out to be the relevant large- $N$  scaling variable. In 4D SU( $N$ ) gauge theories the deconfining transition is first order for  $N \geq 3$  and gets stronger as  $N$  increases.

It is therefore reasonable to conjecture that the  $\theta$  dependence may sharply change right around  $T_c$ , where one may expect a singular behavior, such as a discontinuity.

The purpose of our study is to investigate such a scenario numerically, presenting results for  $N = 3$  and  $N = 6$  to check the  $N$  dependence around the deconfinement transition. The lowest order  $O(\theta^2)$  contribution to the free energy, involving just the topological susceptibility, has been already investigated around the deconfinement transition [9–12]. However, as we shall discuss in detail later on, the study of higher order terms provides a more stringent and definite signature for the change of the  $\theta$  dependence between the two phases. Such a study is the main subject of our investigation.

The finite- $T$  behavior is specified by the free energy

$$F(\theta, T) = -\frac{1}{\mathcal{V}} \ln \int [dA] \exp \left( - \int_0^{1/T} dt \int d^3x \mathcal{L}_\theta \right), \quad (3)$$

where  $T$  is the temperature,  $\mathcal{V} = V/T$  is the Euclidean space-time volume, and the gluon field satisfies  $A_\mu(1/T, \mathbf{x}) = A_\mu(0, \mathbf{x})$ . The  $\theta$  dependence can be parameterized as

$$\mathcal{F}(\theta, T) \equiv F(\theta, T) - F(0, T) = \frac{1}{2} \chi(T) \theta^2 s(\theta, T), \quad (4)$$

where  $\chi(T)$  is the topological susceptibility at  $\theta = 0$ ,

$$\chi = \int d^4x \langle q(x) q(0) \rangle_{\theta=0} = \frac{\langle Q^2 \rangle_{\theta=0}}{\mathcal{V}}, \quad (5)$$

and  $s(\theta, T)$  is a dimensionless even function of  $\theta$  such that  $s(0, T) = 1$ . Assuming analyticity at  $\theta = 0$ ,  $s(\theta, T)$  can be expanded as

$$s(\theta, T) = 1 + b_2(T) \theta^2 + b_4(T) \theta^4 + \dots, \quad (6)$$

where only even powers of  $\theta$  appear.

At zero temperature, where the free energy coincides with the ground-state energy, large- $N$  scaling arguments [2, 13] applied to the Lagrangian (1) indicate that the relevant scaling variable [14] is  $\bar{\theta} \equiv \theta/N$ , i.e.

$$\mathcal{F}(\theta) \approx N^2 \mathcal{G}(\bar{\theta}) \quad (7)$$

TABLE I: Summary of known  $T = 0$  results for the ratio  $\chi/\sigma^2$  (where  $\sigma$  is the string tension) and the first coefficients  $b_{2j}$  for  $N = 3, 4, 6$  [17]. The extrapolation of the results for  $\chi/\sigma^2$ , using the simple Ansatz  $a + b/N^2$ , gives  $\chi/\sigma^2 = 0.022(2)$  for  $N \rightarrow \infty$ . For more complete reviews of results see Refs. [5, 6].

$N$	$\chi/\sigma^2$	$b_2$	$b_4$
3	0.028(2) [5]	-0.026(3) [18–20]	0.000(1) [18]
4	0.0257(10) [21]	-0.013(7) [21]	
6	0.0236(10) [21]	-0.008(4)	0.001(3)

as  $N \rightarrow \infty$ . Comparing with Eq. (4), this implies the large- $N$  behavior

$$\chi = \chi_\infty + O(N^{-2}), \quad b_{2j} = O(N^{-2j}). \quad (8)$$

We recall that a nonzero value of  $\chi_\infty$  is essential to provide an explanation to the  $U(1)_A$  problem in the large- $N$  limit [3, 4]. The apparent incompatibility of Eq. (7) with the periodic nature of the topological  $\theta$  term may be solved by a nonanalytic multibranched  $\theta$  dependence of the ground-state energy [13, 16],  $F(\theta) = N^2 \min_k H\left(\frac{\theta + 2\pi k}{N}\right)$ . The large- $N$  scaling (7) of the  $\theta$  dependence is fully supported by numerical computations exploiting the nonperturbative Wilson lattice formulation of the 4D  $SU(N)$  gauge theory at  $T = 0$ , see, e.g., the results reported in Table I for  $N = 3, 4, 6$  (see also Refs. [5, 6] for recent reviews). This scenario is expected to remain stable against sufficiently low temperatures.

The large- $N$  scaling (7) is not realized by the dilute instanton gas approximation. Indeed, at zero temperature, instanton calculations fail due to the fact that large instantons do not get suppressed. On the other hand, temperature acts as an infrared regulator, so that the instanton-gas partition function is expected to provide an effective approximation of finite- $T$   $SU(N)$  gauge theories at high temperature [15], high enough to make the overlap between instantons negligible. The corresponding  $\theta$  dependence is [15, 22]

$$\mathcal{F}(\theta, T) \approx \chi(T) (1 - \cos \theta), \quad (9)$$

$$\chi(T) \approx T^4 \exp[-8\pi^2/g^2(T)] \sim T^{-\frac{11}{3}N+4}, \quad (10)$$

using  $8\pi^2/g^2(T) \approx (11/3)N \ln(T/\Lambda) + O(\ln \ln T / \ln^2 T)$ . Therefore, the high- $T$   $\theta$  dependence substantially differs from that at  $T = 0$ : the relevant variable for the instanton gas is just  $\theta$ , and not  $\theta/N$ . The instanton-gas approximation also shows that  $\chi(T)$ , and therefore the instanton density, gets exponentially suppressed in the large- $N$  regime, thus suggesting a rapid decrease of the topological activity with increasing  $N$  at high  $T$ . Since the instanton density gets rapidly suppressed in the large- $N$  limit, making the probability of instanton overlap negligible, the range of validity of the instanton-gas approximation is expected to rapidly extend toward smaller and smaller temperatures with increasing  $N$ .

The low- $T$  and high- $T$  phases are separated by a first-order deconfinement transition which becomes stronger with increasing  $N$  [23], with  $T_c$  converging to a finite large- $N$  limit [24]. This suggests the following scenario: the crossover between the low- $T$  large- $N$  scaling  $\theta$  dependence and the high- $T$  instanton-gas  $\theta$  dependence, respectively given by Eqs. (7) and (9), occurs around the deconfinement transition, and becomes sharper and sharper with increasing  $N$ . See, e.g., Refs. [11, 25–27] for further discussions of this scenario.

It is important, at this point, to stress the following: even if the instanton-gas prediction, Eq. (9), receives significant corrections as one approaches  $T_c$  from above, one can still conjecture that the phase transition sharply delimits two regimes with a different large- $N$  scaling behavior, i.e. that the free energy is a function of  $\theta/N$  in the confined phase and a function of  $\theta$  in the deconfined phase. This conjecture is of course more general than the instanton gas picture itself.

The finite- $T$  lattice investigations of the large- $N$  behavior of  $\chi(T)$  [11, 12] indicate a nonvanishing large- $N$  limit for  $T < T_c$ , remaining substantially unchanged in the low- $T$  phase, from  $T = 0$  up to  $T_c$ . Across  $T_c$  a sharp change is observed, and  $\chi(T)$  appears largely suppressed in the high- $T$  phase  $T > T_c$ , in qualitative agreement with a high- $T$  scenario based on the instanton-gas approximation.

However, to achieve a more stringent check of the actual scenario realized in 4D  $SU(N)$  gauge theories, we consider the higher-order terms of the expansion (6), which provide further significant information on the  $\theta$  dependence. Indeed, the expansion coefficients  $b_{2j}$  are expected to scale like  $N^{-2j}$  if the free energy is a function of  $\theta/N$  and to be  $N$ -independent in the instanton-gas approximation. The finite- $T$  behavior of such coefficients has never been studied numerically until now and is the subject of our investigation. In particular, the simple  $\theta$  dependence of Eq. (9) may be observed at much smaller  $T$  above  $T_c$  with respect to the asymptotic one-loop behavior (10) of  $\chi(T)$  which is subject to logarithmic corrections.

In particular, we aim at clarifying: *i*) whether a sharp change in the large- $N$  scaling of  $b_{2j}$  is observed across  $T_c$ , signalling a change from a  $\theta/N$  to a  $\theta$  dependence of the free energy; *ii*) how rapidly the values of  $b_{2j}$  above  $T_c$  converge to the instanton gas prediction, Eq. (9), i.e.

$$b_{2j} = (-1)^j \frac{2}{(2j+2)!}, \quad j = 1, 2, \dots, \quad (11)$$

for the expansion (6). These predictions should be compared to the  $T = 0$  estimates summarized in Table I. It has to be stressed that the results (11) depend just on the form (9) of the free energy and are independent of the renormalized coupling constant  $g(T)$ .

Due to the nonperturbative nature of the physics of  $\theta$  dependence, quantitative assessments of this issue have

largely focused on the lattice formulation of the theory, using Monte Carlo (MC) simulations. However, the complex character of the  $\theta$  term in the Euclidean QCD Lagrangian prohibits a direct MC simulation at  $\theta \neq 0$ . Information on the  $\theta$  dependence of physically relevant quantities, such as the ground state energy and the spectrum, can be obtained by computing the coefficients of the corresponding expansion around  $\theta = 0$ .

We mention that issues related to  $\theta$  dependence, particularly in the large- $N$  limit, can also be addressed by other approaches, such as AdS/CFT correspondence applied to nonsupersymmetric and nonconformal theories, see e.g. Refs. [13, 27–29], and semiclassical approximation of compactified gauge theories [30, 31].

In order to check the change of  $\theta$  dependence across the deconfinement transition, we numerically compute the topological susceptibility and the first few coefficients of the expansion (6) above  $T_c$ , for  $N = 3$  and  $N = 6$  to check the  $N$  dependence. For this purpose we exploit the lattice Wilson formulation of  $SU(N)$  gauge theories

$$S_L = -\frac{\beta}{N} \sum_{x, \mu > \nu} \text{ReTr } \Pi_{\mu\nu}(x), \quad (12)$$

where  $\Pi_{\mu\nu}$  is the standard plaquette operator [32]. The coefficients of the expansion around  $\theta = 0$  can be determined from appropriate zero-momentum correlation functions of the topological charge density at  $\theta = 0$ . These are related to the moments of the  $\theta = 0$  probability distribution  $P(Q)$  of the topological charge  $Q$  and parameterize the deviations of  $P(Q)$  from a simple Gaussian behavior. Indeed [33],

$$\chi_l = \frac{\langle Q^2 \rangle}{L_t L_s^3}, \quad b_2 = -\frac{\langle Q^4 \rangle - 3\langle Q^2 \rangle^2}{12\langle Q^2 \rangle}, \quad (13)$$

$$b_4 = \frac{\langle Q^6 \rangle - 15\langle Q^2 \rangle \langle Q^4 \rangle + 30\langle Q^2 \rangle^3}{360\langle Q^2 \rangle}, \quad (14)$$

where  $\chi_l$  is the the lattice topological susceptibility ( $\chi_l \approx a^4 \chi$ ;  $a$  is the lattice spacing). The correlation functions involving multiple zero-momentum insertions of the topological charge density can be defined in a nonambiguous, regularization independent way [34], and therefore the expansion coefficients  $b_{2i}$  are well defined renormalization-group invariant quantities. This implies that they approach their continuum limit with  $O(a^2)$  corrections.

We evaluate the above quantities in MC simulations for several values of the coupling  $\beta$  on asymmetric  $L_t \times L_s^3$  lattices [35]. Accurate estimates of  $b_{2j}$  require huge statistics, because of the large cancellations when evaluated from the expectation values of powers of  $Q$ , as in Eq. (13). Therefore, we have to consider a relatively fast method to estimate the topological charge  $Q$  of a lattice configuration. We choose the cooling method, and in particular the implementation outlined in Ref. [21]. The

TABLE II:  $N = 3$  results. We report the value of lattice coupling  $\beta$ , the temporal ( $L_t$ ) and spatial ( $L_s$ ) size of the lattice, the reduced temperature  $t \equiv T/T_c - 1$  [38],  $\chi_l$ ,  $\chi/T_c^4$  and the first two coefficients  $b_2$  and  $b_4$  of the expansion (6).

$\beta$	$L_t, L_s$	$t$	$10^5 \chi_l$	$10 \chi/T_c^4$	$-12 b_2$	$360 b_4$
6.173	10, 40	-0.053(3)	2.292(7)	1.84(2)	0.37(12)	-4(11)
6.241	10, 40	0.045(3)	0.645(3)	0.77(1)	1.27(7)	0.7(1.8)
6.273	10, 40	0.095(4)	0.375(3)	0.54(1)	1.15(7)	1.4(1.4)
6.305	10, 40	0.145(6)	0.232(2)	0.40(1)	1.02(5)	3.6(7.2)
6.305	10, 30	0.145(6)	0.233(3)	0.40(1)	1.10(7)	2.9(1.4)
6.437	12, 48	0.147(13)	0.103(3)	0.37(2)	1.07(14)	-1.1(1.4)

TABLE III:  $N = 6$  results. We report the same quantities as in Table II [38].

$\beta$	$L_t, L_s$	$t$	$10^5 \chi_l$	$10^3 \chi/T_c^4$	$-12 b_2$	$360 b_4$
24.797	6, 24	-0.032(10)	17.14(16)	195(8)	0.07(34)	-14(18)
24.912	6, 24	0.045(14)	0.622(13)	9.6(5)	1.15(8)	2.2(1.8)
24.912	6, 20	0.045(14)	0.631(16)	9.8(6)	1.17(8)	2.2(0.7)
25.056	6, 24	0.089(8)	0.132(3)	2.41(9)	1.02(4)	1.0(2)
24.768	5, 20	0.141(7)	0.121(3)	1.28(4)	1.02(2)	1.0(1)
25.200	6, 24	0.160(8)	0.0316(12)	0.74(3)	1.02(4)	1.1(1)

stability of the results under cooling is carefully checked; we take our data after 15 cooling steps, but differences with the results after 10 and 20 cooling steps remain always within the errors reported [36] (for some examples see the appendix). Moreover, the stability substantially improves with increasing  $N$ , as already noted in the literature, also by detailed comparisons with the more rigorous overlap method (which is much more demanding numerically), see, e.g., Ref. [5].

A summary of the results for  $N = 3$  and  $N = 6$  is presented in Tables II and III respectively [37]. The aspect ratio  $L_s/L_t$  in our MC simulations is sufficiently large to give rise to infinite-volume results for the observables considered within the statistical errors, as shown by the comparison of results for different values of  $L_s$ . For the case of both  $SU(3)$  and  $SU(6)$  we check the continuum limit by comparing the results obtained by using two lattices of different temporal extent at the largest value of  $T$ , see Tab. II-III.

The MC results clearly show a change of regime in the  $\theta$  dependence, from a low- $T$  phase where the susceptibility and the coefficients of the  $\theta$  expansion vary very little, to a high- $T$  phase where the coefficients  $b_{2j}$  approach the instanton-gas predictions. Fig. 1 shows the data for  $b_2$ . In the high- $T$  phase they are definitely not consistent with the scaling (8), which would imply a factor of four in  $b_2$ , in going from  $N = 3$  to  $N = 6$ . On the other hand, in the low- $T$  phase  $b_2$  does not significantly differ from the  $T = 0$  value. This is consistent with the behaviour of  $\chi_l$  at  $N = 3$ , for which we obtain:  $\chi_l(T = 0.95T_c)/\chi_l(T = 0) = 0.98(1)$  (at  $\beta = 6.173$ ). A similar behaviour is

observed for  $N = 6$ :  $\chi_l(T = 0.97T_c)/\chi_l(T = 0) = 1.00(2)$  (at  $\beta = 24.797$ ).

Although our MC results in the high- $T$  phase are obtained for relatively small reduced temperatures  $t \equiv T/T_c - 1$ , i.e.  $t < 0.2$ , the data for  $b_2$  show a clear and rapid approach to the value  $b_2 = -1/12$  of the instanton gas model for both  $N = 3$  and  $N = 6$ , with significant deviations visible only for  $t \lesssim 0.1$ . The high- $T$  values of  $b_2$  substantially differ from those of the low- $T$  phase, and in particular from those at  $T = 0$  reported in Table I. Also the estimates of  $b_4$  are consistent with the small value  $b_4 = 1/360$ .

Our data confirm that  $\chi$  rapidly decays with increasing  $t$  in both  $N = 3, 6$  cases. In particular for  $N = 6$  we obtain  $\chi_l(T = 1.09T_c)/\chi_l(T = 0) = 0.0136(4)$  (at  $\beta = 25.056$ ). This suppression is in qualitative agreement with the one-loop instanton-gas result (10), but larger temperatures are required for a reliable quantitative comparison, essentially because of the logarithmic corrections to Eq. (10). The sharp behavior of the  $\theta$  dependence at the phase transition suggests that  $T_c$  is actually a function of  $\theta/N$ , as put forward in Ref. [39].

We have tried to understand the deviations for  $b_2$ , visible at  $t \lesssim 0.1$ , by taking into account corrections to the instanton-gas formula (9) through a virial-like expansion: the asymptotic formula is corrected by a term proportional to the square of the instanton density. For example, we may write

$$\mathcal{F}(\theta, T) \approx \chi(1 - \cos \theta) + \chi^2 \kappa(\theta) + O(\chi^3), \quad (15)$$

where we use the fact that  $\chi(T)$  is proportional to the instanton density, and  $\kappa(\theta)$  can be parametrized as  $\kappa(\theta) = \sum_{k=2} c_{2k} \sin(\theta/2)^{2k}$ . The above formula gives

$$b_2 = -\frac{1}{12} + \frac{1}{8} c_4 \frac{\chi}{T_c^4} + O\left(\frac{\chi^2}{T_c^8}\right). \quad (16)$$

If  $\chi$  gets rapidly suppressed in the high- $T$  phase, as suggested by Eq. (10) and confirmed by the MC results, Eq. (16) would imply a rapid approach to the asymptotic value of the perfect instanton gas, as shown by the data, see Fig. 1. Assuming  $c_4$  weakly dependent on  $N$ , Eq. (16) predicts an exponentially faster convergence with increasing  $N$ , as also supported by the data. Moreover, a hard-core approximation of the instanton interactions [22] gives rise to a negative correction, i.e.  $c_4 < 0$ , explaining the approach from below to the perfect instanton-gas value  $b_2 = -1/12$ .

In conclusion, our numerical analysis provides strong evidence that the  $\theta$  dependence of 4D  $SU(N)$  gauge theory experiences a drastic change across the deconfinement transition, from a low- $T$  phase characterized by a large- $N$  scaling with  $\theta/N$  as relevant variable, to a high- $T$  phase where this scaling is lost and the free energy is essentially determined by the instanton-gas approximation, which implies an analytic and periodic  $\theta$  dependence.

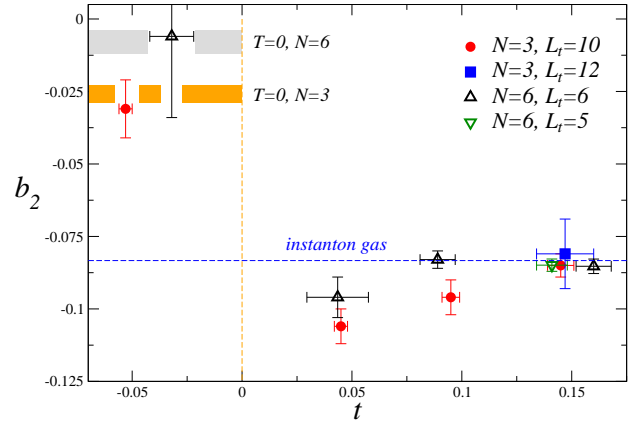


FIG. 1: (Color online) Finite- $T$  results of  $b_2$  for  $N = 3$  and  $N = 6$ , versus the reduced temperature  $t \equiv T/T_c - 1$ . The shadowed regions indicate the  $T = 0$  estimates of  $b_2$  for  $N = 3$  and  $N = 6$ , see Table I.

The corresponding crossover around the transition becomes sharper with increasing  $N$  (see Fig. 1), suggesting that the perfect instanton-gas regime sets in just above  $T_c$  at large  $N$ , while  $\chi(T)$  gets drastically suppressed. A virial-like expansion suggests that the approach is exponential in  $N$ ; this issue deserves further investigation.

It is interesting to remark that hints for an early onset of an instanton gas regime above the chiral/deconfinement transition have been provided by recent MC simulations of full QCD, by looking at the behavior of the relevant susceptibilities [40].

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## APPENDIX: STABILITY ANALYSIS OF THE TOPOLOGICAL MEASUREMENTS

In Fig. (2) and (3) the stability of the results presented in the paper for  $b_2$  and  $b_4$  under cooling is shown:  $n_c$  is the number of cooling steps and  $b_2$  and  $b_4$  are estimated by means of (14), using for the determination of topological charge  $Q$  the prescription of [21]. Figures refer to the case  $t \approx 0.1$ , but all the simulations present similar behaviour.

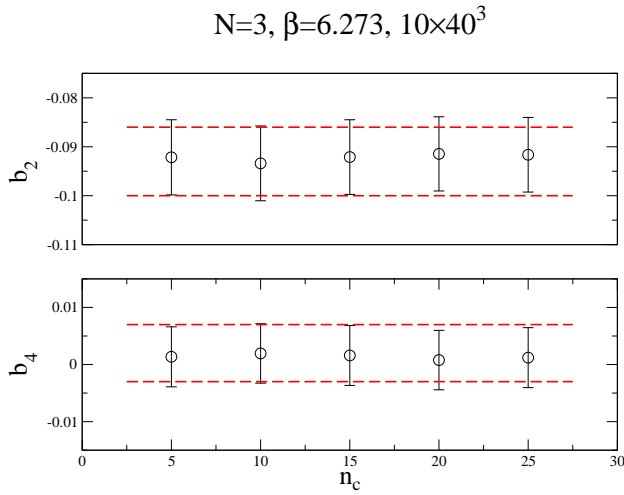


FIG. 2: Results for SU(3).

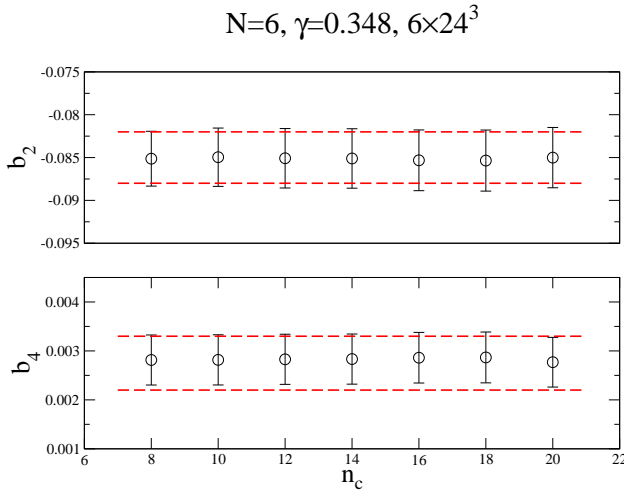


FIG. 3: Results for SU(6).

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- [37] The MC results for  $N = 3$  are obtained by averaging  $O(10^5)$  independent measurements of  $Q$ , corresponding to approximately  $10^7 - 10^8$  sweeps due to the large autocorrelation time  $\tau_Q$  of  $Q$  [21] (e.g.,  $\tau_Q \approx 2 \times 10^3$  for the largest  $\beta$  value,  $\beta = 6.437$ ). In the case of  $N = 6$ , they are obtained from  $O(10^4)$  independent measurements, which corresponds to  $O(10^7)$  sweeps (e.g.,  $\tau_Q \approx 400$  for the runs at  $\beta/(2N^2) = 0.348, 0.350$ ).
- [38] In our analysis, and in particular to determine the reduced temperature, we use results for the transition points at  $N = 3$  taken from Ref. [23]. For the SU(6) gauge theory we use  $\beta_c/(2N^2) = 0.34508(5)$  for  $L_t = 6$  (from [23]),  $\sigma(\beta_c) = 0.276(2)$  and  $t(L_t, \beta) = \sqrt{\frac{\sigma(\beta_c(L_t))}{\sigma(\beta)}} - 1$ .
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